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Light quark masses from unquenched lattice QCD

T. Ishikawa,[1,2] S. Aoki,[3,2] M. Fukugita,[4] S. Hashimoto,[5,6] K-I. Ishikawa,[7]
N. Ishizuka,[1,3] Y. Iwasaki,[3] K. Kanaya,[3] T. Kaneko,[5,6] Y. Kuramashi,[1,3] M. Okawa,[7]
Y. Taniguchi,[1,3] N. Tsutsui,[5] A. Ukawa,[1,3] N. Yamada,[5,6] and T. Yoshié[1,3]
(CP-PACS and JLQCD Collaborations)

[1] *Center for Computational Sciences, University of Tsukuba, Tsukuba 305-8577, Japan*
[2] *RIKEN BNL Research Center, Brookhaven National Laboratory, Upton, New York 11973, USA*
[3] *Graduate School of Pure and Applied Sciences, University of Tsukuba, Tsukuba 305-8571, Japan*
[4] *Institute for Cosmic Ray Research, University of Tokyo, Kashiwa 277-8582, Japan*
[5] *High Energy Accelerator Research Organization (KEK), Tsukuba 305-0801, Japan*
[6] *School of High Energy Accelerator Science, The Graduate University for Advanced Studies (Sokendai), Tsukuba 305-0801, Japan*
[7] *Department of Physics, Hiroshima University, Higashi-Hiroshima 739-8526, Japan*

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We calculate the light meson spectrum and the light quark masses by lattice QCD simulation, treating all light quarks dynamically and employing the Iwasaki gluon action and the nonperturbatively $O(a)$-improved Wilson quark action. The calculations are made at the squared lattice spacings at an equal distance $a^2 \simeq 0.005$, 0.01 and 0.015 fm^2, and the continuum limit is taken assuming an $O(a^2)$ discretization error. The light meson spectrum is consistent with experiment. The up, down and strange quark masses in the $\overline{\rm MS}$ scheme at 2 GeV are $\overline{m} = (m_u + m_d)/2 = 3.55^{+0.65}_{-0.28}$ MeV and $m_s = 90.1^{+17.2}_{-6.1}$ MeV where the error includes statistical and all systematic errors added in quadrature. These values contain the previous estimates obtained with the dynamical u and d quarks within the error.

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The masses of light quarks are fundamental parameters of QCD. They cannot be measured experimentally since quarks are confined in hadrons. Lattice QCD enables calculations of hadron masses as functions of quark masses, and hence allows a determination of the quark masses from the experimental hadron masses. This approach has been successfully applied, first in quenched QCD [1] and then in $N_f = 2$ QCD where degenerate up (u) and down (d) quarks are treated dynamically [2]. These studies have revealed that the light quark mass values are significantly reduced by dynamical u and d quark effects. In this article, we present our attempt to determine the quark masses in $N_f = 2 + 1$ QCD where the heavier strange (s) quark is also treated dynamically. We wish to examine to what extent the dynamical s quark affects the light quark masses. We determine the quark masses in the continuum limit and estimate all possible systematic errors. We also calculate the prerequisite light meson spectrum. A similar attempt has been made by the MILC Collaboration [3].

We adopt the Iwasaki RG gauge action [4] and the clover quark action with the improvement coefficient c_{SW} determined nonperturbatively for the RG action [5]. The choice of the gauge action is made to avoid a first-order phase transition (lattice artifact) observed for the plaquette gauge action [6]. We employed the Wilson quark formalism because we prefer an unambiguous quark-flavor interpretation over the computational ease of the staggered formalism adopted by the MILC collaboration [7].

Configurations are generated at three values of the coupling $\beta \equiv 6/g^2 = 2.05, 1.90$ and 1.83 corresponding to the squared lattice spacing $a^2 \simeq 0.005, 0.01$ and 0.015 fm^2, with the physical volume fixed to about (2.0fm)^3. At each β, we perform simulations for 10 quark mass combinations using a combined algorithm [8] of the Hybrid Monte Carlo (HMC) for the degenerate u and d quarks and the polynomial Hybrid Monte Calro (PHMC) for the s quark. Table I summarizes the simulation parameters.

The meson and quark masses at the simulation points are determined from single exponential correlated χ^2 fits to the correlators $\langle P(t)P(0)\rangle$, $\langle V(t)V(0)\rangle$ and $\langle A_4(t)P(0)\rangle$, where P, V and A_μ denote pseudoscalar, vector and nonperturbatively $O(a)$-improved [9] axial-vector current operators, respectively. We use an exponentially smeared source and a point sink, and measurements are made at every 10 HMC trajectories in the Coulomb gauge. For the pseudoscalar sector, $\langle P(t)P(0)\rangle$ and $\langle A_4(t)P(0)\rangle$ are fitted simultaneously ignoring correlations among them. Errors are estimated by the jackknife method with a bin size of 100 HMC trajectories; errors do not increase for larger bin sizes.

Chiral fits are made to the light-light (LL), light-strange (LS) and strange-strange (SS) meson masses simultaneously ignoring their correlations, using a quadratic polynomial function of the sea quark masses (m_u, m_d, m_s) and valence quark masses $(m_{\rm val1}, m_{\rm val2})$ in mesons;

$$\begin{aligned} & f(\mathrm{M_s}, \mathrm{M_v}) \qquad (1) \\ = \; & A + B_S \mathrm{tr}\mathrm{M_s} + B_V \mathrm{tr}\mathrm{M_v} + D_{SV} \mathrm{tr}\mathrm{M_s}\mathrm{tr}\mathrm{M_v} \\ & + C_{S1}\mathrm{tr}\mathrm{M_s^2} + C_{S2}(\mathrm{tr}\mathrm{M_s})^2 + C_{V1}\mathrm{tr}\mathrm{M_v^2} + C_{V2}(\mathrm{tr}\mathrm{M_v})^2, \end{aligned}$$

where $f = m_{PS}^2$ or vector meson mass m_V, $\mathrm{M_S} =$

TABLE I: Simulation parameters; $L^3 \times T$ is the lattice size, (κ_{ud}, κ_s) is the hopping parameter combination, $1/\delta\tau$ is the number of molecular dynamics steps in one trajectory, $N_{\rm poly}$ is the PHMC polynomial order, and traj. is analyzed trajectory length. Pseudoscalar vector mass ratios $\frac{m_{\rm PS}}{m_{\rm V}}$ are also listed for light-light (LL) and strange-strange (SS) mass combinations.

κ_{ud}	κ_s	$\delta\tau$	$N_{\rm poly}$	traj.	$\frac{m_{\rm PS}}{m_{\rm V}}$(LL)	$\frac{m_{\rm PS}}{m_{\rm V}}$(SS)	κ_{ud}	κ_s	$\delta\tau$	$N_{\rm poly}$	traj.	$\frac{m_{\rm PS}}{m_{\rm V}}$(LL)	$\frac{m_{\rm PS}}{m_{\rm V}}$(SS)
$\beta = 1.83,\ L^3 \times T = 16^3 \times 32,\ c_{SW} = 1.761$													
0.13655	0.13710	1/80	80	7000	0.7772(13)	0.7522(15)	0.13655	0.13760	1/90	110	7000	0.7769(14)	0.7235(19)
0.13710		1/85	80	7000	0.7524(21)	0.7524(21)	0.13710		1/100	110	8600	0.7448(14)	0.7128(16)
0.13760		1/100	100	7000	0.7076(18)	0.7414(17)	0.13760		1/110	120	8000	0.7033(18)	0.7033(18)
0.13800		1/120	110	8000	0.6629(22)	0.7365(16)	0.13800		1/120	130	8100	0.6525(23)	0.6941(20)
0.13825		1/140	120	8000	0.6213(24)	0.7343(15)	0.13825		1/150	150	8100	0.6083(32)	0.6884(21)
$\beta = 1.90,\ L^3 \times T = 20^3 \times 40,\ c_{SW} = 1.715$													
κ_{ud}	κ_s	$\delta\tau$	$N_{\rm poly}$	traj.	$\frac{m_{\rm PS}}{m_{\rm V}}$(LL)	$\frac{m_{\rm PS}}{m_{\rm V}}$(SS)	κ_{ud}	κ_s	$\delta\tau$	$N_{\rm poly}$	traj.	$\frac{m_{\rm PS}}{m_{\rm V}}$(LL)	$\frac{m_{\rm PS}}{m_{\rm V}}$(SS)
0.13580	0.13580	1/125	110	5000	0.7673(15)	0.7673(15)	0.13580	0.13640	1/125	140	5200	0.7667(16)	0.7211(21)
0.13610		1/125	110	6000	0.7435(18)	0.7647(17)	0.13610		1/125	140	8000	0.7444(15)	0.7182(17)
0.13640		1/140	110	7600	0.7204(19)	0.7687(15)	0.13640		1/140	140	9000	0.7145(16)	0.7145(16)
0.13680		1/160	110	8000	0.6701(27)	0.7673(17)	0.13680		1/160	140	9200	0.6630(21)	0.7127(17)
0.13700		1/180	110	7900	0.6390(22)	0.7691(15)	0.13700		1/180	140	7900	0.6243(28)	0.7102(20)
$\beta = 2.05,\ L^3 \times T = 28^3 \times 56,\ c_{SW} = 1.628$													
κ_{ud}	κ_s	$\delta\tau$	$N_{\rm poly}$	traj.	$\frac{m_{\rm PS}}{m_{\rm V}}$(LL)	$\frac{m_{\rm PS}}{m_{\rm V}}$(SS)	κ_{ud}	κ_s	$\delta\tau$	$N_{\rm poly}$	traj.	$\frac{m_{\rm PS}}{m_{\rm V}}$(LL)	$\frac{m_{\rm PS}}{m_{\rm V}}$(SS)
0.13470	0.13510	1/175	200	6000	0.7757(26)	0.7273(29)	0.13470	0.13540	1/175	250	6000	0.7790(23)	0.6821(32)
0.13510		1/195	200	6000	0.7316(24)	0.7316(24)	0.13510		1/195	250	6000	0.7341(29)	0.6820(39)
0.13540		1/225	200	6000	0.6874(30)	0.7395(23)	0.13540		1/225	250	6000	0.6899(34)	0.6899(34)
0.13550		1/235	200	6500	0.6611(34)	0.7361(25)	0.13550		1/235	250	6500	0.6679(45)	0.6899(43)
0.13560		1/250	200	6500	0.6337(38)	0.7377(28)	0.13560		1/250	250	6500	0.6361(47)	0.6852(46)

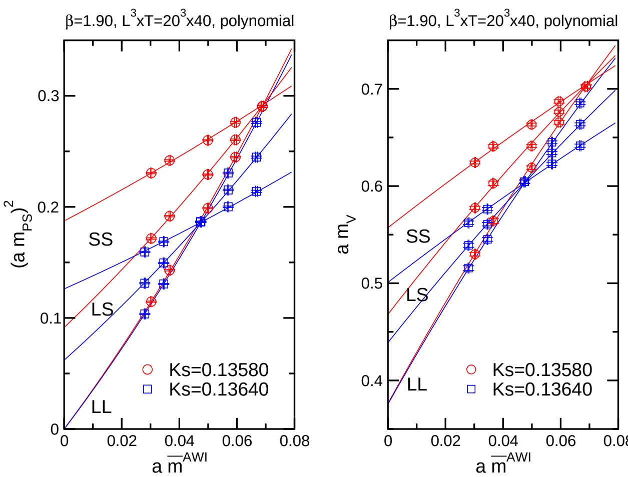

FIG. 1: Chiral fits of meson masses with m_q^{AWI} at $\beta = 1.90$.

$\mathrm{diag}(m_u, m_d, m_s)$, $\mathrm{M_V} = \mathrm{diag}(m_{\rm val1}, m_{\rm val2})$, and "tr" means the trace of matrices. In the fits, we use the axial-vector Ward identity quark mass $m_q = \lim_{t\to\infty}\langle \partial_4 A_4(t) P(0)\rangle / (2\langle P(t)P(0)\rangle)$ and set $A = B_S = C_{S1} = C_{S2} = 0$ for m_{PS}^2. These fits reproduce measured data well, as illustrated in Fig.1, with reasonable χ^2/d.o.f. of at most 1.36.

The physical quark mass point and the lattice spacing are determined from the experimental values of π^0, ρ^0 and K (K-input) or π^0, ρ^0 and ϕ (ϕ-input) meson masses. Taking the ρ^0 mass as input may cause a large systematic error, because the $\rho \to \pi\pi$ decay mode is not open for our mass range (the lightest pion mass in this simulation ~ 620 MeV) and hence chiral extrapolation of m_V for lighter quarks may be quite different from our fits. In order to estimate this uncertainty, we also check another combination $[\pi^0, K, \phi]$. We assume the ideal mixing for the vector isosinglets. Since our simulation is made with degenerate u and d quarks, we consider the isospin averages $m_{\hat{K}} = \{(m_{K^\pm}^2 + m_{K^0}^2)/2\}^{1/2}$ and $m_{\hat{K}^*} = (m_{K^{*\pm}} + m_{K^{*0}})/2$ and predict the average light quark mass $\overline{m} = (m_u + m_d)/2$. The electromagnetic (EM) effects, not included in our simulations, are removed from the $m_{K^\pm}$ above using Dashen's theorem [10] $(m_{K^\pm}^2 - m_{K^0}^2)_{\rm EM} = (m_{\pi^\pm}^2 - m_{\pi^0}^2)_{\rm EXP}$. The isospin breaking effects and the EM effects for other mesons we consider are expected to be small and thus are not considered. The experimental values we use are taken from the PDG booklet [11]; $m_{\pi^0} = 0.1350$GeV, $m_{\pi^\pm} = 0.1396$GeV, $m_{K^0} = 0.4976$GeV, $m_{K^\pm} = 0.4937$GeV, $m_{\rho^0} = 0.7755$GeV, $m_{K^{*0}} = 0.8960$GeV, $m_{K^{*\pm}} = 0.8917$GeV and $m_\phi = 1.0195$GeV. Lattice spacings (Table II) for the K- and ϕ- inputs are consistent, while those for the $[\pi, K, \phi]$-input are slightly smaller by at most 7%.

TABLE II: Lattice spacings in fm units.

β	K-input	ϕ-input	$[\pi, K, \phi]$-input
1.83	0.1174(23)	0.1184(26)	0.1095(25)
1.90	0.0970(26)	0.0971(25)	0.0936(33)
2.05	0.0701(29)	0.0702(28)	0.0684(41)

An agreement of the meson spectrum with experiment is a necessary condition for a reliable estimate of the quark masses. To confirm this, we extrapolate the me-

TABLE III: Meson masses in the continuum limit (in MeV units), compared to experiment. The EM effect is subtracted using Dashen's theorem.

	K-input	ϕ-input	$[\pi, K, \phi]$-input	EXP.
$\hat{K}$	-	491(19)	-	495.0
ρ^0	-	-	761(32)	775.5
$\hat{K}^*$	900.5(9.9)	898.0(1.4)	891(16)	893.9
ϕ	1025(19)	-	-	1019.5

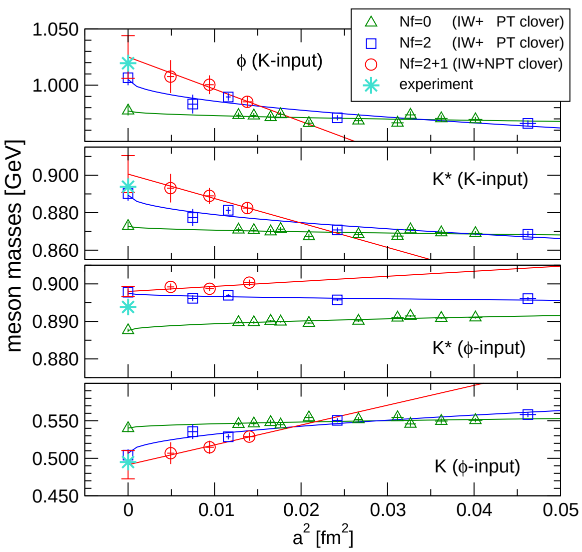

FIG. 2: Continuum extrapolation of meson masses for $N_f = 2+1$ QCD (circles), compared to experiment (stars) and results in $N_f = 2$ (squares) and $N_f = 0$ (triangles) QCD [2].

son masses linearly in a^2, because our action is $O(a)$ improved and data are well fitted, as shown in Fig.2, with small $\chi^2/\text{d.o.f} \leq 1.4$. The masses in the continuum limit, summarized in Table III, are consistent with experiment with at most 2.9σ deviation. The $\hat{K}^*$ mass turns out to be slightly heavier than experiment, though the supplemental $[\pi, K, \phi]$-input gives consistent results with experiment with large statistical error. Possible origin of the deviation is due to uncertainty of chiral fits. In fact, an alternative fit based on chiral perturbation theory (χPT) we discuss later yields $m_{\hat{K}^*} = 894(12)$ MeV (K-input). In Fig.2 we overlay the previous results of meson masses [2] in the $N_f = 2$ and quenched ($N_f = 0$) QCD with tadpole improved one-loop c_{SW}. The dynamical u and d quarks significantly reduce the $O(10\%)$ deviation of the quenched spectrum from experiment. We find no further dynamical s quark effect beyond statistical errors.

The quark masses are evaluated for the $\overline{\text{MS}}$ scheme at the scale $\mu = 2\text{GeV}$ using the tadpole improved one-loop matching [12] at $\mu = a^{-1}$ with an improved coupling determined from plaquette and rectangular loop and four-loop renormalization group equation. In the continuum extrapolation of the quark masses, we assume

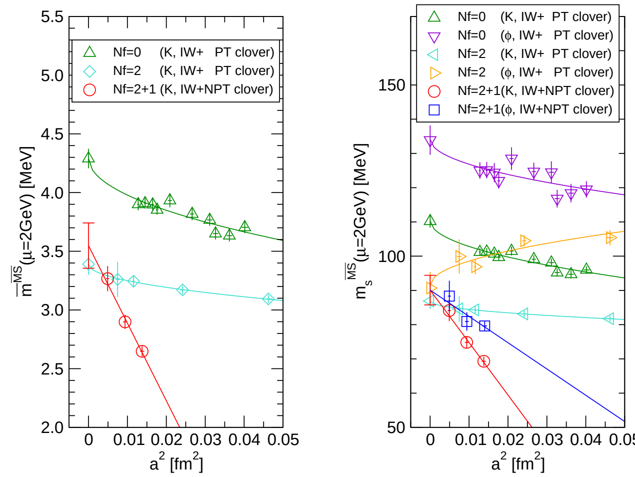

FIG. 3: Continuum extrapolations of the up, down and strange quark masses. For comparison, results for $N_f = 0$ and $N_f = 2$ QCD [2] are overlaid.

the $O(g^4 ma)$ contributions are small and neglect it. As Fig. 3 shows, the quark masses are well described by a linear function in a^2, and the values determined for either the K- or the ϕ-inputs, while different at finite lattice spacings, extrapolate to a common value in the continuum limit. Therefore the continuum limit is estimated from a combined linear fit with the K- and the ϕ-inputs. We obtain $\overline{m}^{\overline{\text{MS}}}(\mu = 2\text{GeV}) = 3.55(19)$ MeV and $m_s^{\overline{\text{MS}}}(\mu = 2\text{GeV}) = 90.1(4.3)$ MeV with a sufficiently small $\chi^2/\text{d.o.f.} < 0.42$. Note that the supplemental $[\pi, K, \phi]$-input gives larger statistical error and hence is not used to estimate central values.

We now turn to estimates of possible systematic errors. **Finite size effect (FSE)** — The meson masses at the infinite volume are estimated at $\beta = 1.90$ using data on a $V \sim (2.0\text{fm})^3$ lattice and those from our exploratory study on a $V \sim (1.6\text{fm})^3$ lattice [13], and assuming a strong volume dependence of $(m_{\text{had},V} - m_{\text{had},V=\infty})/m_{\text{had},V=\infty} \propto 1/V$ [14]. The chiral fits to the infinite volume values lead to less than a 4% change for the meson masses at the physical point. For the quark masses, however, we find a larger shift of 12.2% from a $V \sim (2.0\text{fm})^3$ lattice to $V = \infty$ for $\overline{m}$ with ϕ-input and 8.1% for m_s with K-input (differences are smaller for the other cases). Assuming that FSE is independent of lattice spacing, we take the differences as estimates of FSE for the quark masses in the continuum limit.

Chiral extrapolation — In addition to the polynomial chiral fits, we fit the meson masses using χPT formulaes modified for the Wilson quark action (WχPT) [15]. Namely, we fit m_π, $m_{\hat{K}}$, m_ρ and $m_{\hat{K}^*}$ using the NLO $N_f = 2+1$ QCD WχPT formulae for the $O(a)$ improved theory [16]. Since the formula in Ref. [16] is not applicable for the ϕ meson, we estimate the effect only for K-input. In the fits we obtain $\overline{m}$ to be 3.1% smaller and m_s to be 1.2% larger than those of the polynomial fit. We note that our WχPT fits to data do not exhibit a clear

chiral logarithm, probably because u and d quark masses in our simulation are not sufficiently small. Further possible systematic error from a long chiral extrapolation for ρ^0, mentioned above, is estimated by the supplemental $[\pi, K, \phi]$-input, which gives 3.0% larger for $\overline{m}$ and 3.4% larger value for m_s than the central one. For an estimate of systematic errors from chiral fits, differences of the two alternative fits from the central value are added linearly.
Renormalization factor — Uncertainty of the one-loop calculation of the renormalization factor is estimated by shifting the matching scale from $\mu = 1/a$ to $\mu = \pi/a$ and also using an alternative tadpole improved coupling [2].
Continuum extrapolation — Possible $O(a^3)$ effects are investigated by performing the continuum extrapolation adding an $O(a^3)$ term to the fit function.
Electromagnetic (EM) effects — Systematic error due to uncertainty of the EM effects is estimated following extensive arguments [7, 17, 18] to Dashen's theorem [10]. Namely, we estimate the effects by a further mass shift of our input $m_{\hat{K}}$ using a relation $(m^2_{K^\pm} - m^2_{K^0})_{\rm EM} = (1 + \Delta_E)(m^2_{\pi^\pm} - m^2_{\pi^0})_{\rm EXP}$ assuming the EM effects for other mesons are negligeble. We vary the Δ_E in range $[-1, +1]$ as our estimate of the EM effects, and we find a quite small change in m_s and no change in $\overline{m}$.
Isospin breaking effects — Isospin breaking effects are estimated by chiral fits with Eq. (1) for $m_u \neq m_d$ and taking m_{π^0}, m_{ρ^0}, $m_{K^\pm}$ and m_{K^0} as inputs. We find that $m_u/m_d = 0.577(25)$, and that $\overline{m}$ and m_s have no change from the $\hat{K}$ input result. We note that m_u/m_d strongly depends on an estimate of the EM effects; m_u/m_d =0.663–0.498 for $\Delta_E = [-1, +1]$, though $\overline{m}$ and m_s almost do not.

Finally we obtain

$$\overline{m}^{\overline{\rm MS}}(\mu = 2{\rm GeV}) = 3.55(19)(^{+43}_{-0})(^{+11}_{-11})(^{+26}_{-17})(^{+34}_{-0})(^{+0}_{-0})(^{+0}_{-0}), \quad (2)$$

$$m_s^{\overline{\rm MS}}(\mu = 2{\rm GeV}) = 90.1(4.3)(^{+7.3}_{-0})(^{+4.2}_{-0})(^{+6.6}_{-4.3})(^{+12.8}_{-0})(^{+0.1}_{-0.2})(^{+0}_{-0}), \quad (3)$$

in MeV units, where the errors are statistical, systematic due to FSE, chiral extrapolation, renormalization factor, continuum extrapolation, EM effect and isospin breaking effect, respectively. Adding the errors in quadrature yields the values quoted in the abstract. These values agree well with the latest report from the MILC Collaboration [3] $\overline{m} = 3.3 \pm 0.3$ MeV and $m_s = 90 \pm 6$ MeV where we added the quoted errors in quadrature. They also include the $N_f = 2$ values [2] within the error.

Scaling violation in the quark masses is unexpectedly large, while that for the meson masses are reasonably bounded at a percent level at $a \approx 0.1$ fm. To gain a better control over systematic uncertainties, a significant reduction in the simulated light quark masses on a correspondingly larger lattice is needed. An attempt is underway to meet these challenges [19].

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